chapter #3 notes :-

Electronegetivity :-

Definition :- Power of an atom to attact shared pair of electrons towards itself in a molecule.

H — Cl

Trends along Group :- It decreases from top to bottom in the group.

Reasons :

- Atomic size increase
- Shielding increase
- Nuclear charge decrease which means that attraction of es with nucleus decreases.

Halogens ;

decrease E.N.

F (4.0)
Cl (3.1)
Br (2.9)
I (2.6)
At (rare)

Trends along period :- Increases along the period.

Atomic size decreases

Nuclear charge increase which means attraction of es with nucleus increase.

Shielding effect remains constant.

VIII A has highest E.N as Grap IIIA has its octet complete so it does not form bond.

Nature of bond :- | Purpose of Electronegativity.

→ E.N tells us about nature of bond whether it's ionic or covalent.

→ $\Delta E.N = E_2 - E_1$ (Difference of E.N)

→ If $\Delta E.N$ is greater (>) than 1.8 → ionic

→ If $\Delta E.N$ is smaller (<) than 1.8 → covalent

Non-polar (0 - 0.4) | polar (0.4 - 1.8)

Dipole moment :- → Polarity of Bond.

formula ⇒ $\mu = q \times r$

→ Product of Magnitude of charge and distance b/w them. (vector)

→ It is directed from + pole to - pole

Application / Purpose :-

→ Measurement of polarity of Bond.

→ if $\mu = 0$, then non-polar compound] e.g; Benzene

if $\mu \neq 0$, then polar compound] chlorobenzene $\mu = 1.2D$

e.g;

$q = 1.6022 \times 10^{-19} C$

So, $\mu = q \times r$

$= 1.6022 \times 10^{-19} \times 2.5 pm$

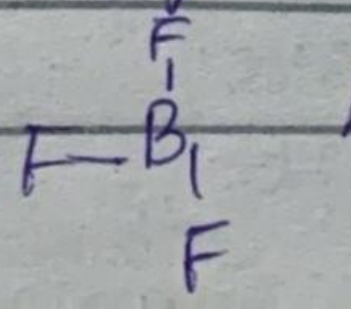
Note; All linear Structure have $\mu = 0$:-

Structure whose angles are 180° are linear structure :

O = C = O , S = C = S

↓ net force = 0

→ All trigonal planar structure have $\mu = 0$



$\mu = 0$

Bond energy :-

→ Amount of energy required to break 1 mol of bond. **OR**

→ Amount of energy released when 1 mol of bond is formed from it's element under Standard condition ↓. ΔH°

under ⇒ 1 atm pressure
298K / 25°C → Temproom

→ It can be exothermic or endothermic.

Example :-

① $\underset{(H_2)\ \text{molecule}}{H \overset{}{-} H} \longrightarrow \underset{\text{atom}}{H} + H \quad \Delta H = 436\ kj/mol.$

→ endothermic → absorb energy
rxn

→ exothermic rxn → Released energy.

② $\underset{\text{molecule}}{Cl \overset{}{-} Cl} \longrightarrow \underset{\text{atoms}}{Cl} + Cl \quad \Delta H = +243\ kj/mol$

OR

⇒ Exothermic

① $\underset{\text{atom}}{H} + H \longrightarrow H_2 \quad \Delta H = -436\ kj/mol$

② $\underset{\text{atom}}{Cl} + Cl \longrightarrow Cl_2 \quad \Delta H = -243 kj/mol$

Conclusion :-

→ Bond formation release energy
→ Bond breaking absorb energy.

⇒ Factors effecting bond energy :-

① E.N Difference ∝ polarity ∝ Bond Strength ∝ Bond energy
→ Difference will make bond strong and high amount of energy is needed to break bond.

HF > HCl > HBr > HI → decrease.
(1.9) (0.8) (0.7) (0.4) B.E

② Size of Bonded atom $\propto \frac{1}{B.E}$

(3) Bond length :-

Distance between two bonded atom.

$B.L \propto \frac{1}{B.E}$

e.g; Amstrong

C–C 1.54A° → C=C 1.34A° → C≡C 1.20A°

C–H = 1.07A° more B.E

C–C = 1.54A° less B.E

(4) Bond order :- $\propto B.E$

⇒ No. of bond form by atom

→ Unit ; Kj/mol

① VSEPR Theory

Valance Shell Electron pair repulsion Theory.

Postulates :

(1) Central atom arrange the electron pair in a such a way that there is maximum distance blw the eletrons pair.

e.g;
AB_2 → B–A–B (180° → they will show repulsion.)
type

central atom ($2\bar{e}$ pair)

Atom in a molecule in which other atoms are attached, it can be, 180°, 120°, 90°

AB_3 → (B, A, B, B; 360°) (Trigonal planar)
type

(2)

Repulsion order b/w Electron pair, (jitna smaller bond hoga utna repulsion hogi).

lone-lone pair > lone pair > Bond pair → more repel.
Decreasing order; small Bond pair

∴ Repulsion $\alpha \frac{1}{\text{angle}}$ ⇒ If repulsion b/w two atoms is greater than angle will be smaller.

CH_4	NH_3
109.5	107

⇒ If repulsion b/w two atoms is smaller b/c than angle will be greater.

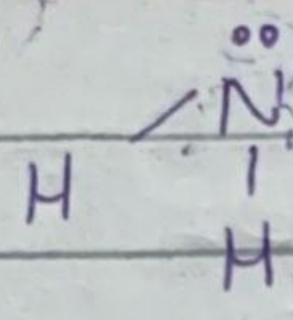
E.g; AB_2 ($\frac{1}{2}$) AB_3 ($\frac{1}{3}$) AB_4 ($\frac{1}{4}$)

$AB_4 > AB_3 > AB_2$.

The lone pair causes deviation from ideal bond angle.

(3) lone pair occupy more space as compared to bond pair.

e.g;



120°, 100°, 90°

→ trigonal pyrimidal

(4) Both lone pair and bond pair determine the geometry of the molecules. or

Final Geometry of molecules depend upon no. of electron pair and nature of e pair.

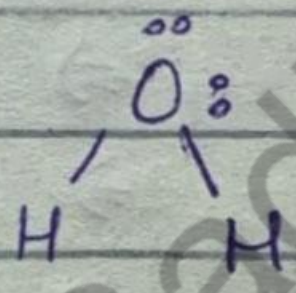
e.g;

AB_2 type 2 e pair linear pair → AB_3 type 3 ē pair trigonal pair → AB_4 type 4 election pair tetrahedral.

e.g; $\ddot{N}H_3$

3 B.P + 1 L.P = 4 → trigonal

H_2O ⇒



2 L.P = 4 Angular

2 B.P < 109.5

(5) Double bond and triple bond is considered to be one electron pair / single bond.

C=C ↓ 2 pair of ē

C≡C ↓ 3 pair of ē

Bond pair	lone pair
This consist of ~~pair~~ two electrons shared b/w two atoms. depend upon of shared ē pair. ⇒ They help to achieve stability and complete valance shell.	This a pair of electrons that are localized on a single atom and are not shared with other atoms.

Applications of VSEPR theory :

(2) $BeCl_2$:-

Type : AB_2

Total $\bar{e}$ pair = 2

Bond pair = 2

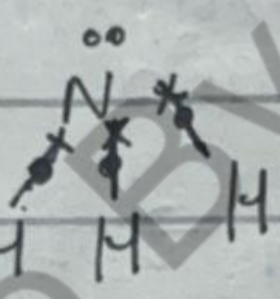
lone pair = 0

$\bar{e}$ pair geometry = Linear

(Shape of Molecule / Geometry of Molecule) = Linear

Angle = 180°

(3) NH_3



Type : AB_3E

Total $\bar{e}$ pair = 4

Bond pair = 3

lone pair = 1

$\bar{e}$ pair Geometry = Tetrahedral

Final Geometry = Trigonal pyrimidal

Angle = < (less than) 109.5

(4) $AlBr_3$

Types = AB_3

$\bar{e}$ Total pair = 3

Bond pair = 3

lone pair = 0

$\bar{e}$ pair Geometry = Trigonal planer

final Geometry = Trigonal planer

Angle :- 120°

(5) PCl_3

Type = AB_3E

$\bar{e}$ pair = 4

Bond pair = 3

lone pair = 1

valance bond theory (VBT) :-

Postulates :-

① A bond b/w two atoms is formed by overlap of half-filled atomic of two atoms. These orbitals retain there identity. e.g; p^6 , [p^5, p^4, p^3, p^2, p^1]

H ① Cl ① → half filled/ incomplete.

HCl

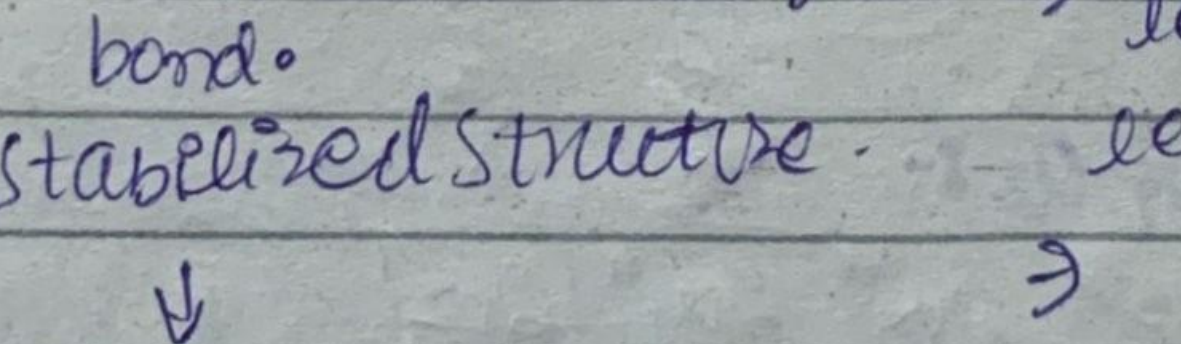
(3) Bond formed ∝ unpaired electron. e.g; p_x^1 p_y^1 p_z^1

(4) By the overlapping of 2 orbital a single → first bond. bond which ⁂ sigma bond is formed.

P_x — P_x → first bond σ

→ By the overlapping of additional orbital multiple bond are formed. ⇒ = (π bond)

(5) - In order to form bond the overlapping orbital must have same symmetry.



(6.) Energy is released by overlaping of orbitals.

Bond → Energy → atom stable.

released

→ more overlapping ↲ energy released stronger bond.

→ stabilized structure.

↓

⇒ more.

overlapping ∝ energy released.

↓

→ less overlapping

less energy weak bond.

⇒ instable compairtively

→ less

• The energy of atomic orbital is high before overlapping.

8-

② $HgCl_2$
⇒ AB_2
⇒ 2
⇒ 2
⇒ 0
⇒ linear
⇒ Linear

⇒ 180°

SH_2
= AB_2E_2
= 4
⇒ 2
⇒ 2
⇒ Tetrahedral
⇒ Bent
⇒ 104°

⑤ $SiCl_4$
= AB_4
= 4
= 4
= 0
= Tetr
= Tet
= 10

etry = Te
met = T

8 8
• minimum overlappe
• Small Bond energy
• High Bond length.
• maximum overlapping
• High Bond energy

valance bond theory (VBT) 8-

Postulates 8-

① A bond b/w two atoms is formed by overlap of half-filled atomic of two atoms. These orbitals retain there identity. e.g; p^6 ,[p^5, p^4, p^3, p^2, p^1]

H ① Cl ①

half filled/ incomplete.

① HCl

(3) Bond formed ∝ unpaired electron. e.g; p_x^1 p_y^1 p_z^1

(4) By the overlapping of 2 orbital a single → first bond which sigma bond is formed.

Px Px → first bond σ

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Px axis Px

Y Z X

same Symmetry

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Bond → Energy → atom stable.

released

overlapping ∝ energy released.

→ more overlapping ↵ energy released stronger bond.
→ stabilized structure.
⇓
→more.

→ less overlapping less energy release
⇒ instable bond.
compairtively
→ less

The energy of atomic orbital is high before overlapping.

Types of overlapping :→ refers to interaction of atomic orbital when atoms bond together.

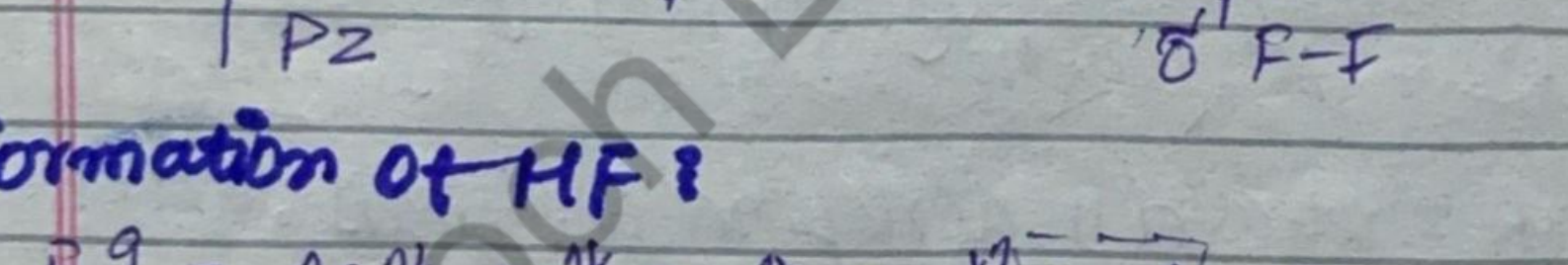
① Sigma bond
② Pi bond (π)

① **Sigma bond :-** when there is a single bond blw 2 atom • formed between ; ① S-S , ② S-Px ③ S-Py , ④ S-Pz (Direct contact)

② Pi bond (π) → 2nd overlap (2nd bond blw 2 atom)
3rd overlap

→ Pi bond is formed b/w parallel.

① Py - Py ② Pz - Pz

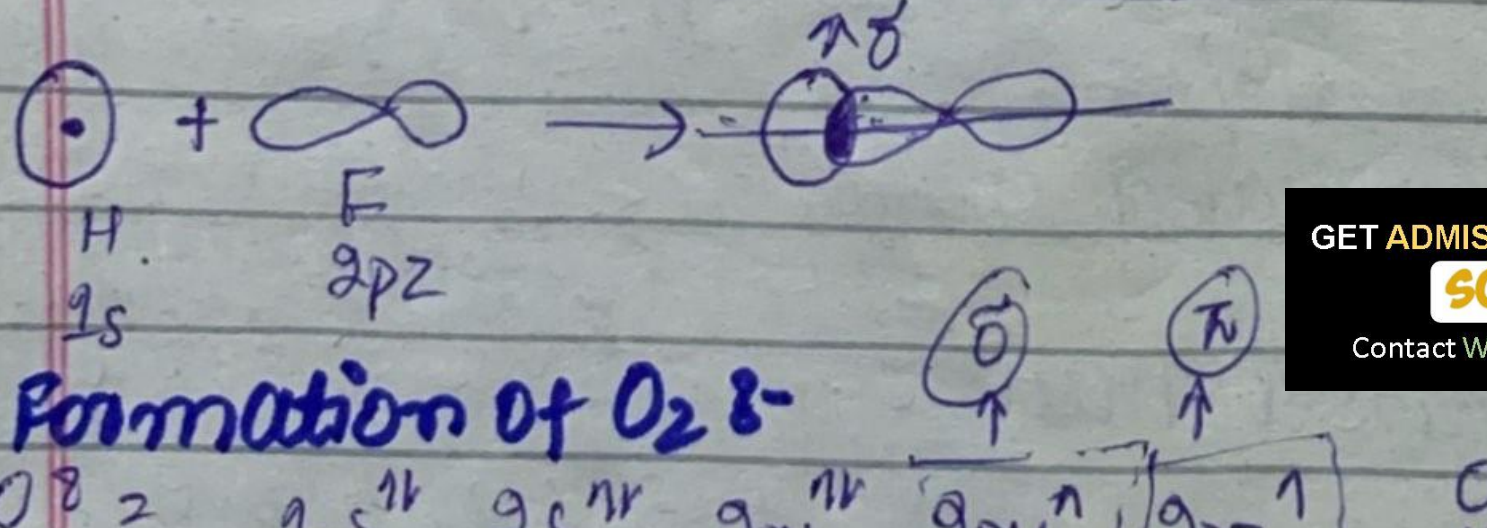


Application of VBT :-

② **Formation of F_2 :-**

F^9 = $1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2px^{\uparrow\downarrow}\ 2py^{\uparrow\downarrow}\ 2pz^{\uparrow}$

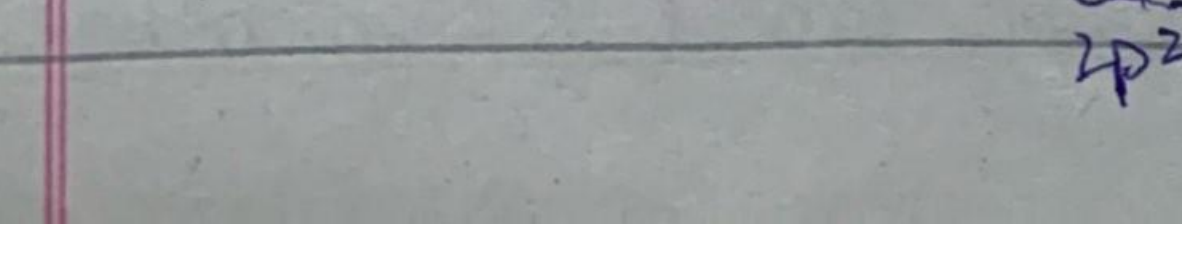
F^9 $1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2px^{\uparrow\downarrow}\ 2py^{\uparrow\downarrow}\ 2pz^{\uparrow}$ → first bond



③ **Formation of HF :**

F^9 = $1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2px^{\uparrow\downarrow}\ 2py^{\uparrow\downarrow}\ 2pz^{\uparrow}$ F

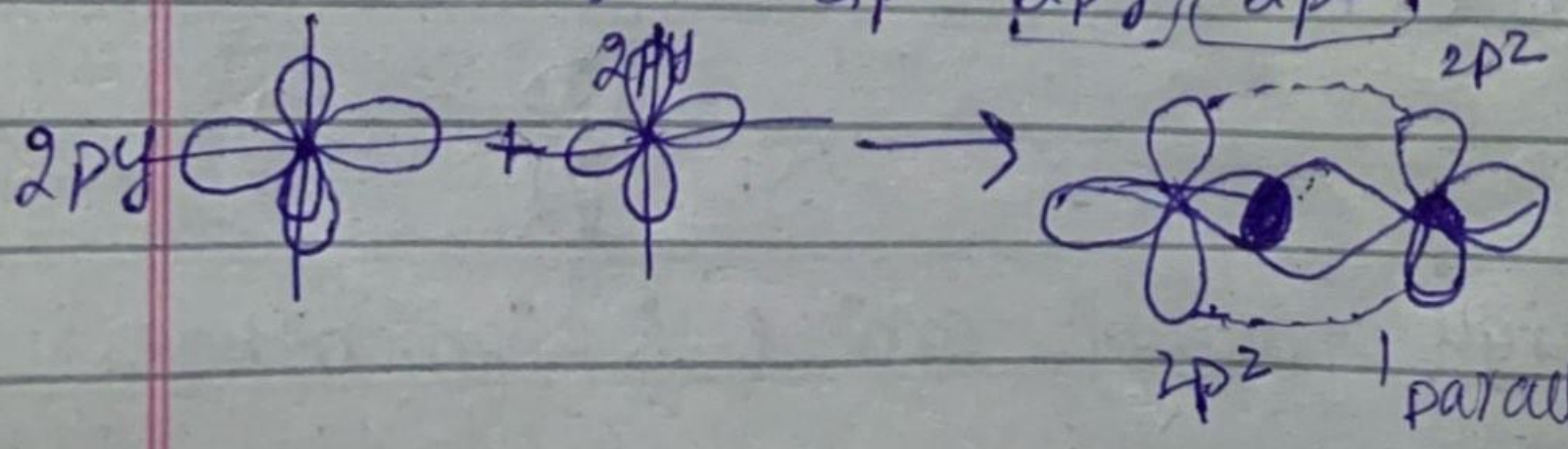
H^1 = $1s^{\uparrow}$ H

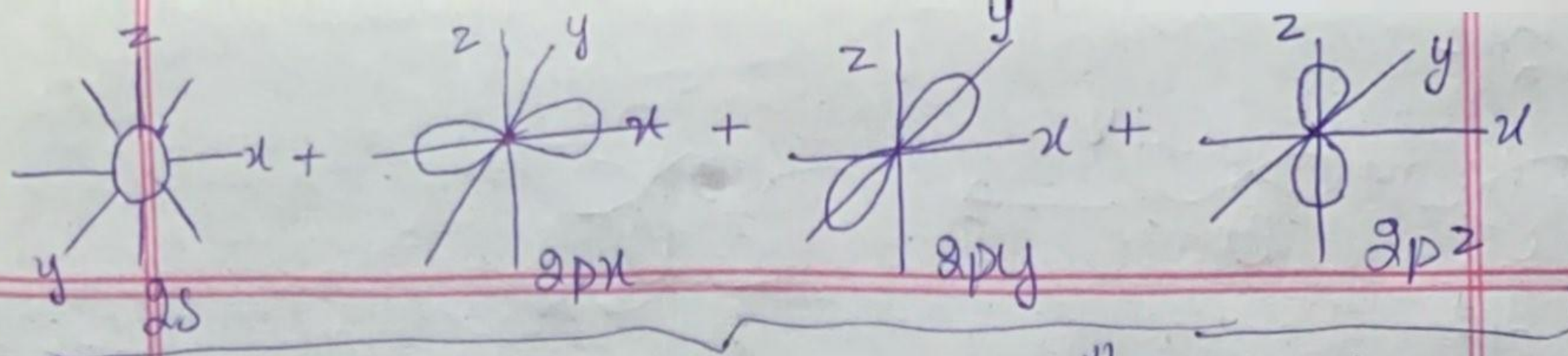


③ **Formation of O_2 :-**

O^8 = $1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2px^{\uparrow\downarrow}\ 2py^{\uparrow}\ 2pz^{\uparrow}$ O

O^8 = $1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2px^{\uparrow\downarrow}\ 2py^{\uparrow\downarrow}\ 2pz^{\uparrow\downarrow}$ O





unhybrid orbital.

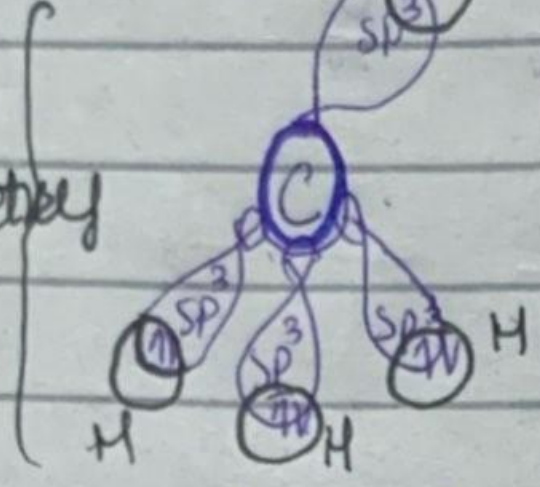
↓

hybrid orbitals

sp^3 sp^3 sp^3 sp^3

CH_4 Molecular Geometry :

final Geometry



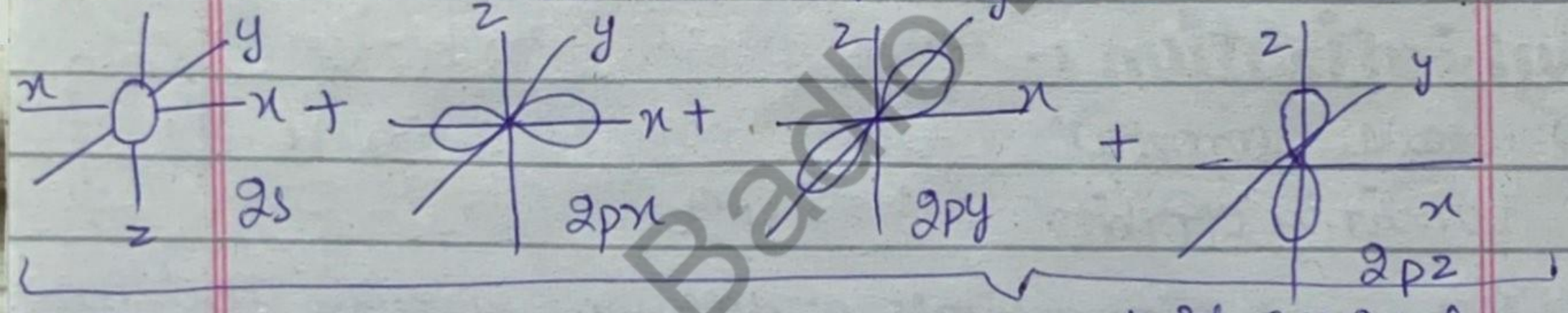
- Tetrahedral (109°5)
- σ bond = 4

(2) NH_3 One s and three 2p orbital form 4 sp^3 orbital

N^{7} 8- $1s^{2}$ $2s^{2}$ $2px^{1}$ $2py^{1}$ $2pz^{1}$ Groond state

N^{7} 8 $1s^{2}$ [2] [1] [1] [1]

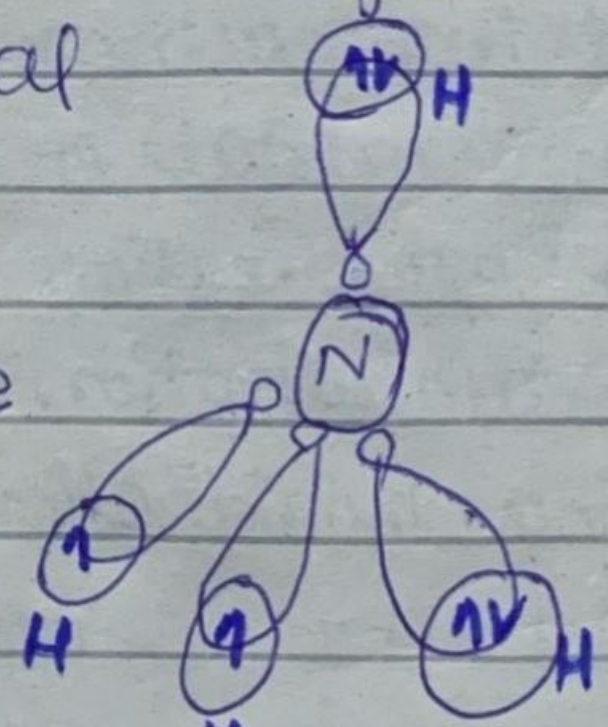
2s Px Py Pz



unhybrid orbital

↓

4 4 4 4 hybrid orbital



Findl geometry :-

Trigonal pyramid Molecule

(107·5)

σ bond = 4

(3) Ethane (C_2H_6)

$C^{6} \rightarrow$ $1s^{2}$ $2s^{2}$ $2Px^{1}$ $2Py^{1}$ $2Pz$ Ground state

$C^{6} \rightarrow$ $1s^{2}$ $2s^{1}$ $2px^{1}$ $2py^{1}$ $2pz^{1}$ Excited state

$C^{6} \Rightarrow$ $1s^{2}$ [1] [1] [1] [1] → hybrid

2s 2px 2py 2pz state.

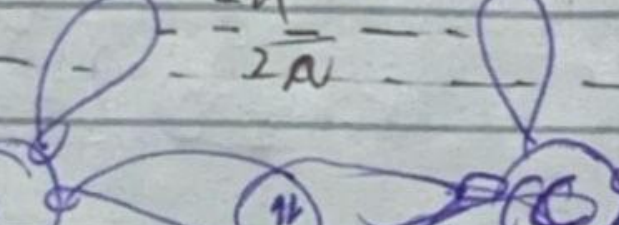
sp^3 sp^3 sp^3 sp^3

Examples: $BeCl_2$

$Be = 1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2p_x^{\uparrow}\ 2p_y\ 2p_z$ Ground state

$Be = 1s^{\uparrow\downarrow}\ 2s^{\uparrow}\ 2p_x^{\uparrow}\ 2p_y\ 2p_z$ excited state

$1s^{\uparrow\downarrow}$ [↑ ↑] $2p_y\ 2p_z$ hybrid state



180°
linear

C_2H_2

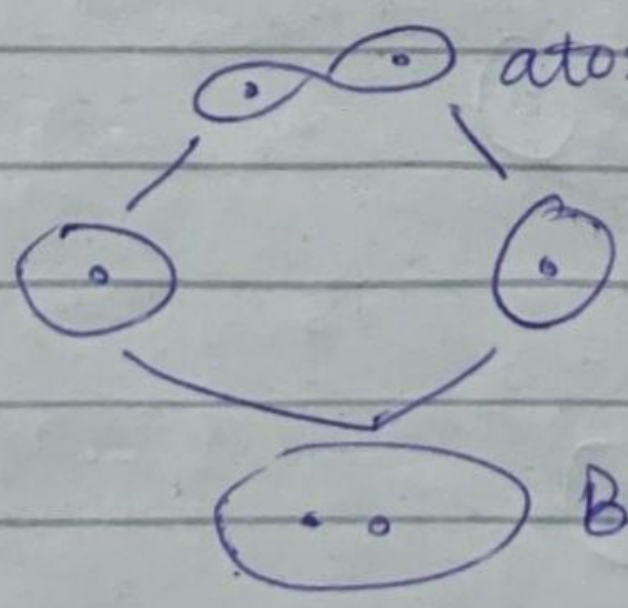
$C^6 = 1s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2p_x^{\uparrow}\ 2p_y^{\uparrow}\ 2p_z$ grandstate

$C^6 = 1s^{\uparrow\downarrow}\ 2s^{\uparrow}\ 2p_x^{\uparrow}\ 2p_y^{\uparrow}\ 2p_z^{\uparrow}$

[↑ ↑]
2s 2px

Molecular orbital Theory:-

Statement:- According to this theory linear combination of atomic orbital form new orbital called molecular orbital.



↓

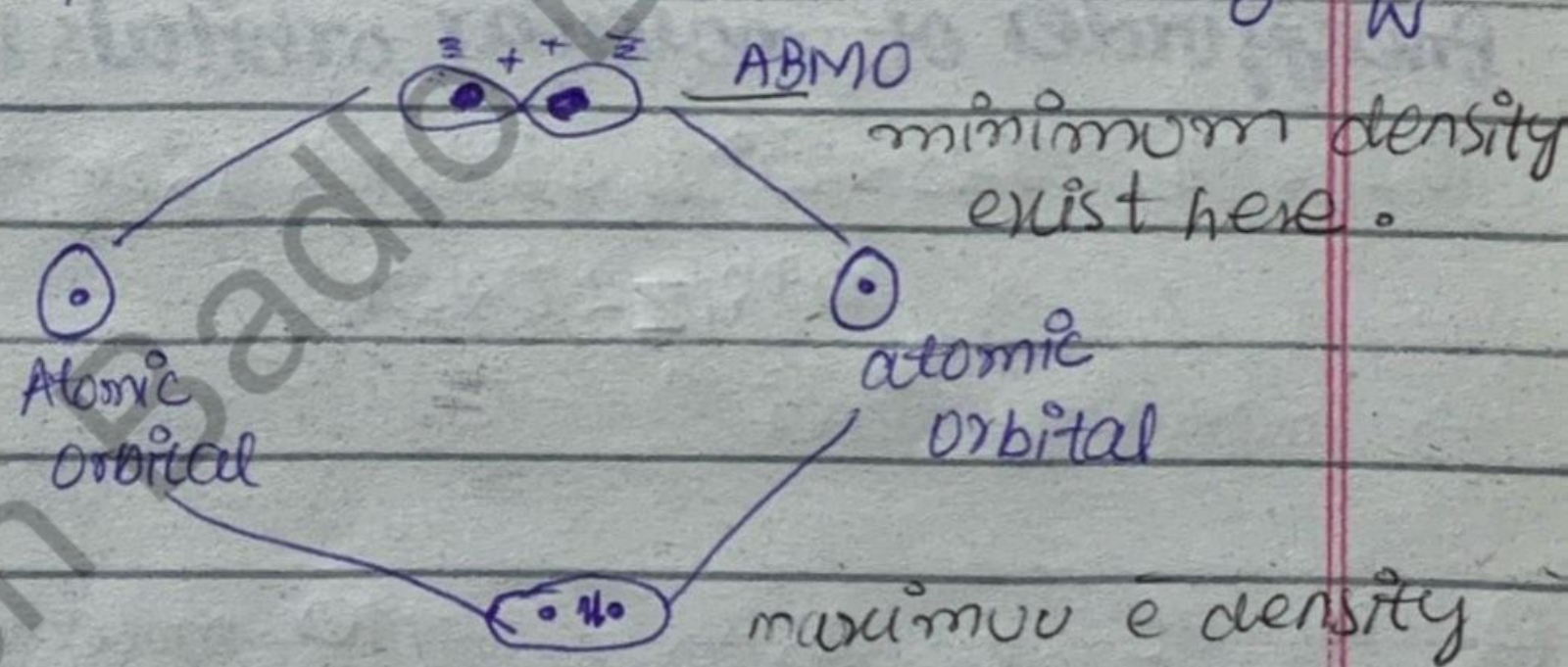
Have less energy than atomic orbital.

atomic orbital → Molecular orbital — A·B·M·O – high energy
B·M·O – low energy

1. During this process the identity of atomic orbitals are lost.
2. After the combination of atomic orbital different type of ~~atomic~~ molecular orbitals are formed which are different in energy.
   (1) Bonding molecular orbital (of lower energy)
   (2) Antibonding molecular orbital (Higher energy)

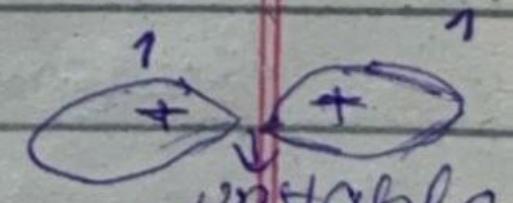
Bonding Molecular orbital :-

→ They have low energy but high density.
→ They are formed by overlapping of orbitals (atomic)
→ BMO has high ē density blw the two nucleus which is responsible for stable bond.

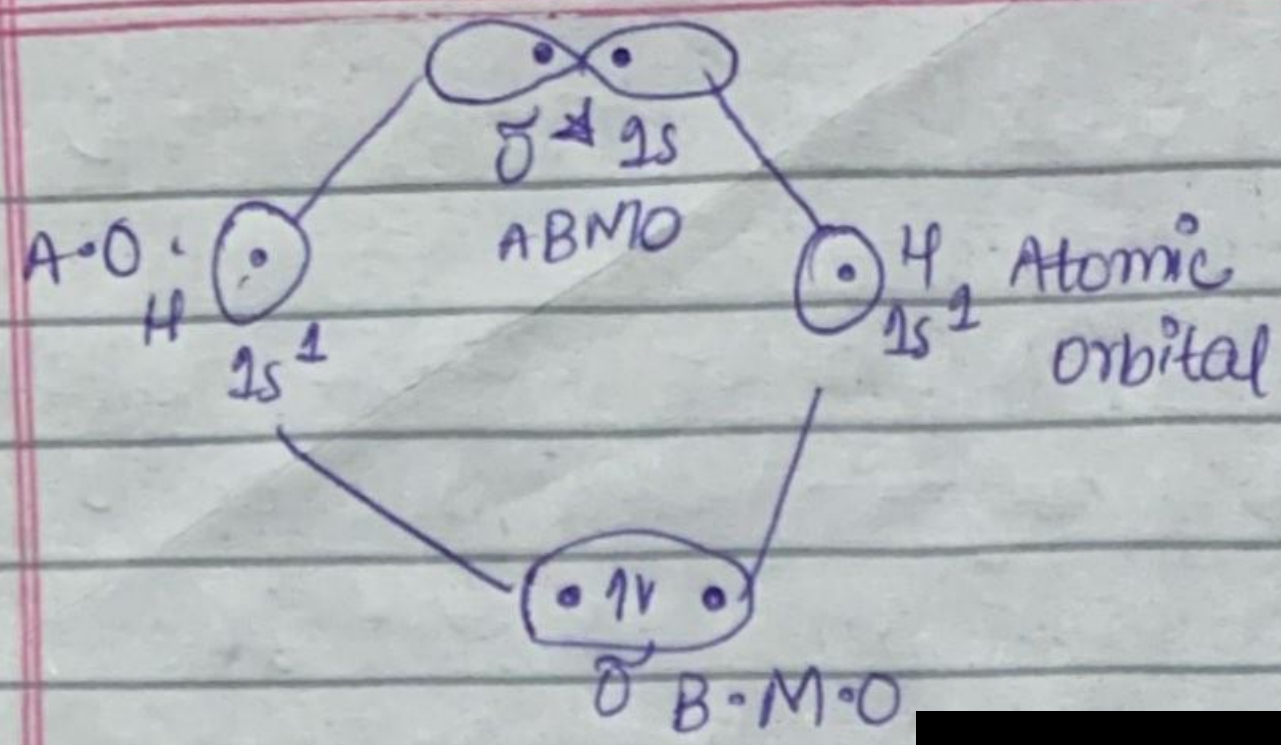
→ 

Antibonding orbital :-

→ They have zero density and high energy.
→ They are formed by substraction of atomic overlap orbital
→ It has zero ē density blw the two nucleus which is responsible for unstable bond.
→ Each ē of ABMO contribute to repulsion blw atoms. , σ* π*



S → overlapping σS σ*S



Py − Py , P2 − P2

↓ π | π

πpy = πpz

Energy order of filling orders :-

$\underbrace{\sigma 2p_x}_{B.M.O} > \pi 2p_y = \pi 2p_z > \underbrace{\pi^* 2p_y = \pi^* 2p_z}_{ABMO} > \sigma^* 2p_x$

opposite energy

Energy order of molecular orbitals :- O_2, F_2 and their ions.

$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_x < \pi 2p_y = \pi 2p_z < \pi^* 2p_y = \pi^* 2p_z < \sigma^* 2p_x$

→ increasing order of energy

② H_2, Be_2, B_2, C_2, N_2 (lighter molecules)

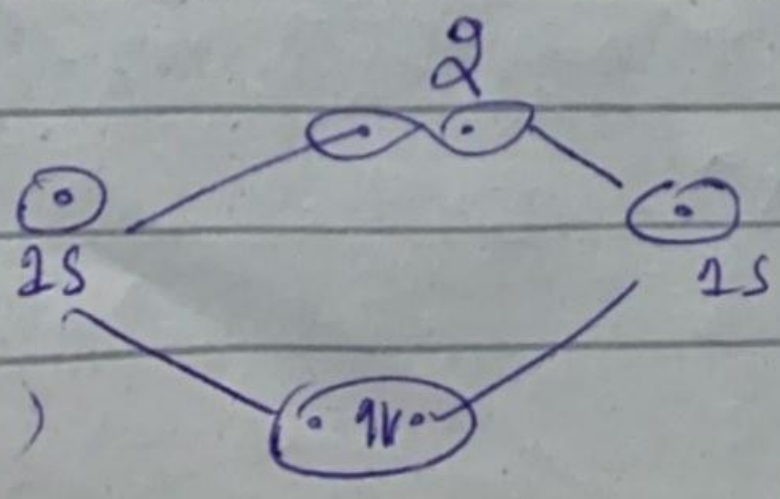
$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \pi 2p_y = \pi 2p_z < \sigma 2p_x > \pi^* 2p_y = \pi^* 2p_z < \sigma^* 2p_x$

Bond Order :-

Statement :- Total no. of bonds formeds when two atoms overlap each other.

B.O = no. of $\bar{e}$ BMO − no. of $\bar{e}$ AB MO

e.g;

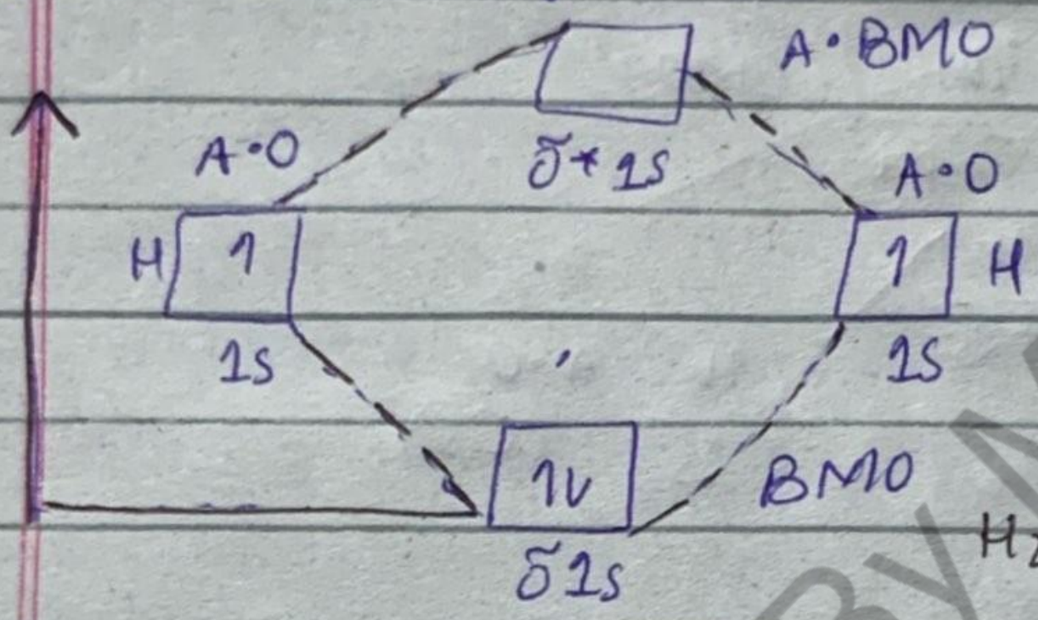


$= \frac{2-0}{2} = 1$

→ Element having unpaired $\bar{e}$ called paramagnetic
→ Element having paired $\bar{e}$ called dimagnetic.

→ If Bond order is negative than bond does not exist
→ and if it is zero than bond does not exist.
→ Positive valle of order means that bond is stable.

Application of MOT :-



$B.O = \frac{2-0}{2} = 1$

H is — unpaired $\bar{e}$ so dimagnetic.

$H_2 = \sigma 1s^2, \sigma^* 1s^0$

→ Bond order 1 means that there is a single bond b/w them. Magnesium :-

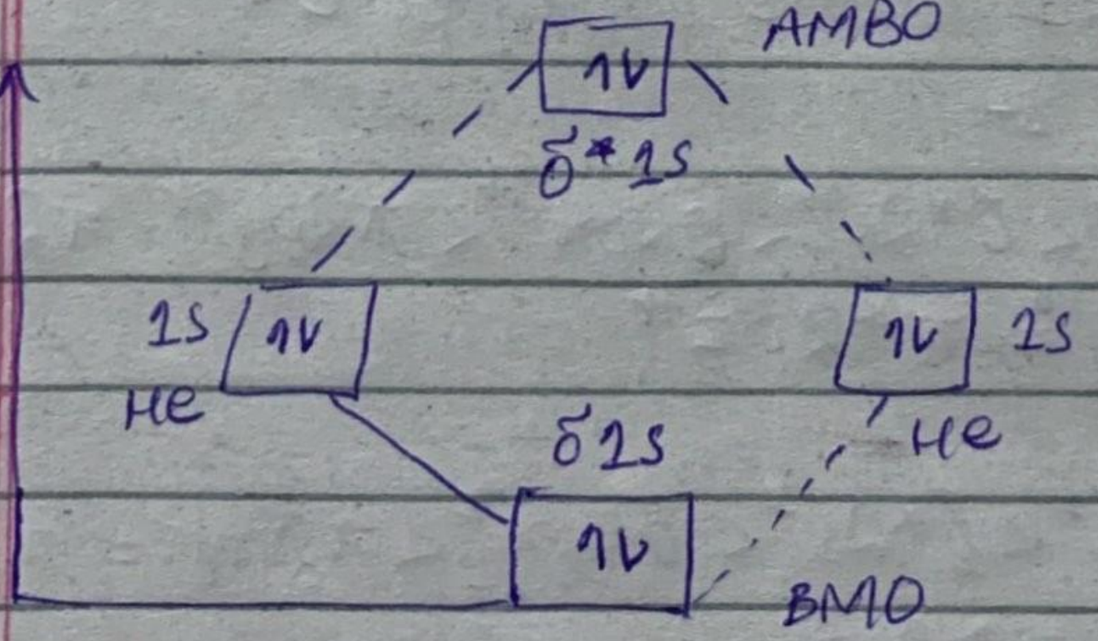
- H has single bond and it has no unpaired $\bar{e}$ so it is dimagnetic.

Electronic configaration according to MOT :-

$H_2 = \sigma 1s^2, \sigma^* 1s$

Formation of He_2 :-

$1s^2$



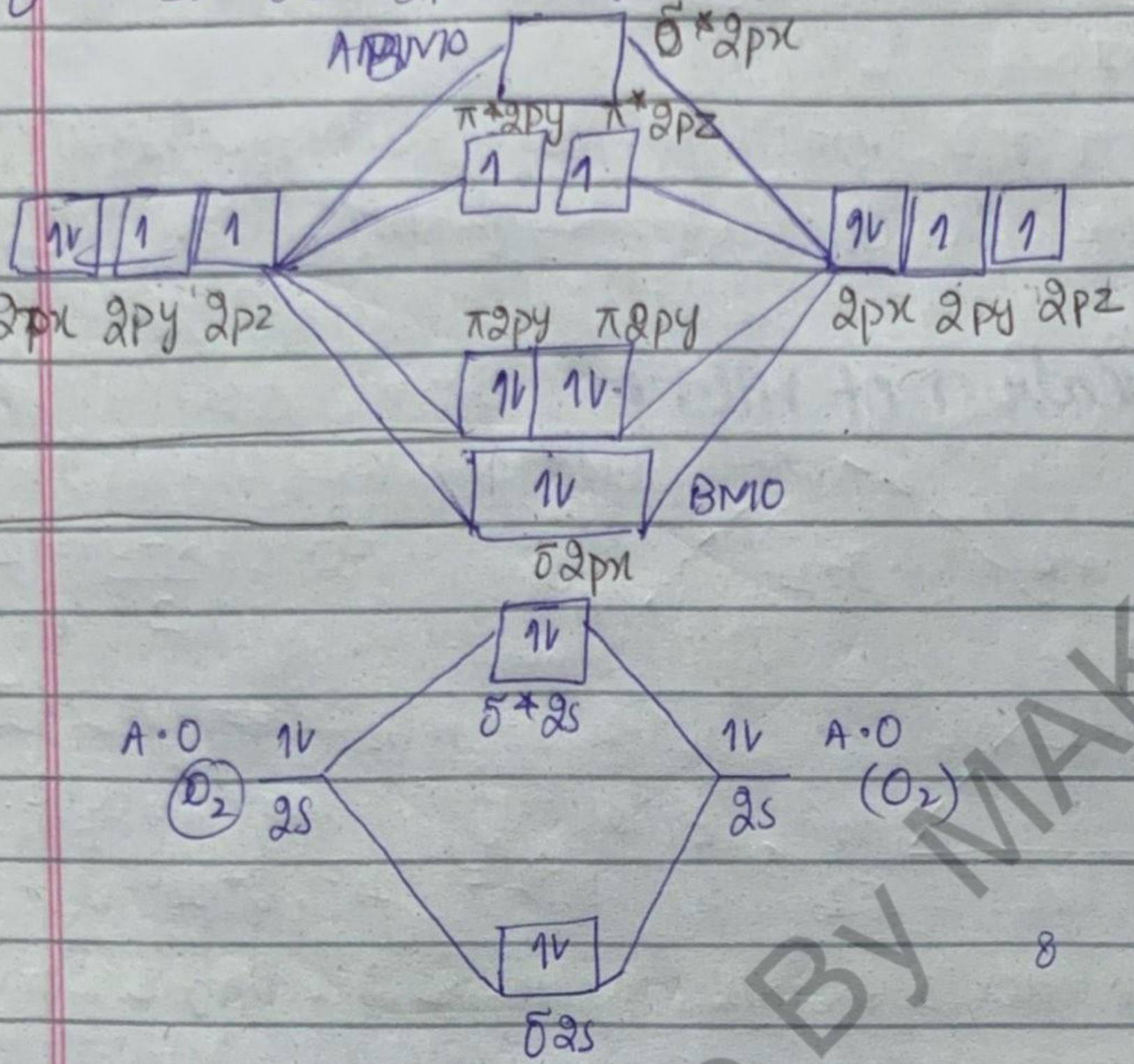
$B.O = \frac{2-2}{2} = 0$

→ this bond does not exist.

$He = \sigma 1s^{1v}, \sigma^* 1^{1v}$

Formation Of O_2 :-

$O^8 = 2s^{\uparrow\downarrow}\ 2s^{\uparrow\downarrow}\ 2px^{\uparrow\downarrow}\ 2py^{\uparrow}\ 2pz^{\uparrow}$



$\sigma 1s > \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2px < \pi 2py = \pi 2pz < \pi^* 2py = \pi^* 2pz < \sigma^* 2px$

Bond order :- $\frac{8-4}{2} = 4/2 = 2$

→ O will be form double bond with otheratom

Magnesium :-

Paramagnetic bc2 it one unpairede⁻.

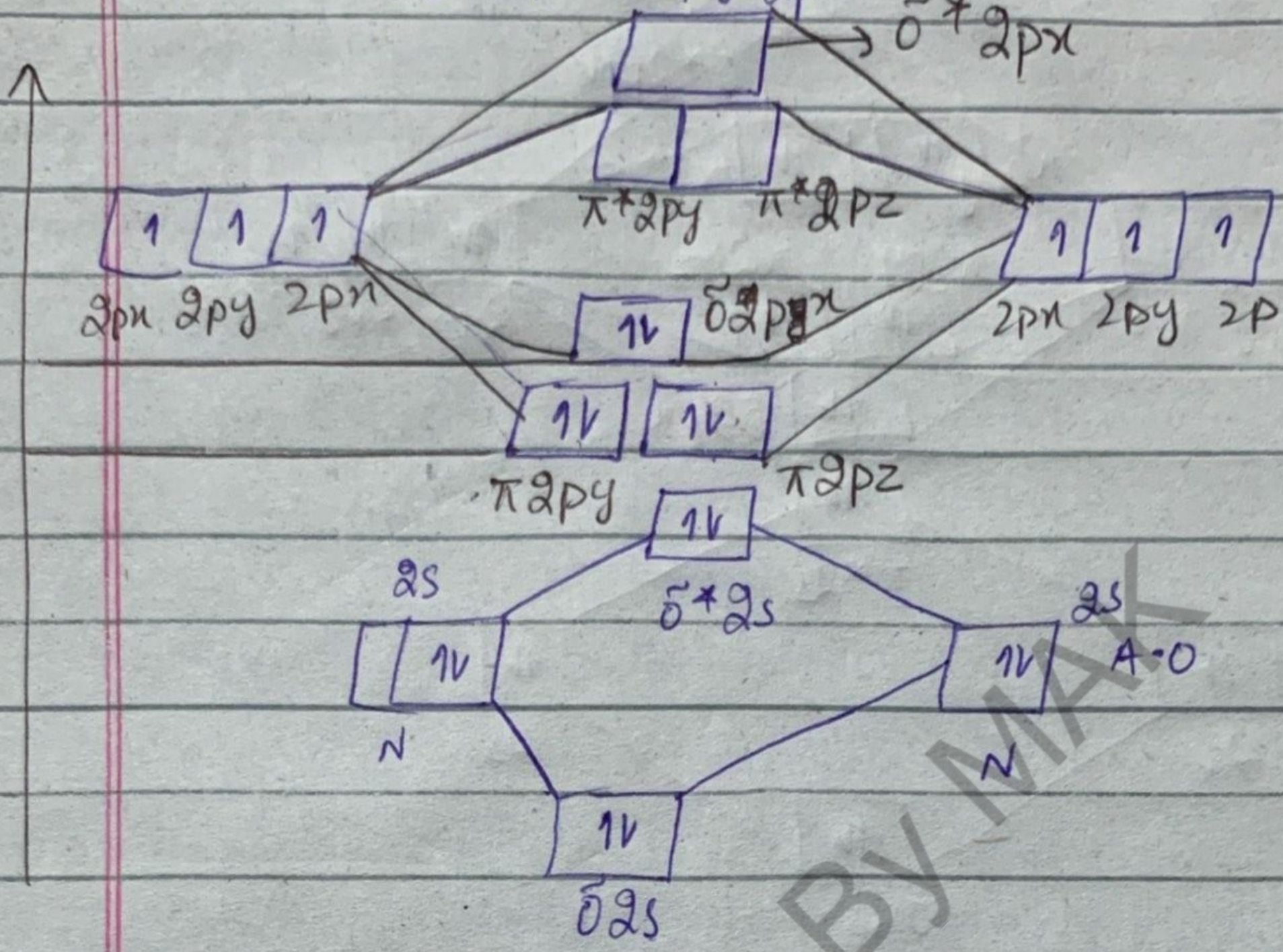
EC according to MOT :-

$\sigma 1s^{\uparrow\downarrow} < \sigma^* 1s^{\uparrow\downarrow} < \sigma 2s^{\uparrow\downarrow} < \sigma^* 2s^{\uparrow\downarrow} < \sigma 2px^{\uparrow\downarrow} < \pi 2py^{\uparrow\downarrow} = \pi 2py^{\uparrow\downarrow} < \pi^* 2py^{\uparrow} = \pi^* 2pz^{\uparrow}$

$\Rightarrow \sigma 1s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2 < \sigma 2px^2 < \pi 2py^2 = \pi 2pz^2 < \pi^* 2py^2 = \pi^* 2pz^2.$

Formation of N_2 :-

$N^7 = 1s^{\uparrow\downarrow} 2s^{\uparrow\downarrow} 2p_x^{1} 2p_y^{1} 2p_z^{1}$



Bond order = $\frac{8-2}{2} = 6/2 = 3$

→ Triple Bond exist blw nitrogen atoms.

Magnesium :- Diamagnetic

Electronic configaration of MOT :-

$N^7 =$

$\sigma 2s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2 < \pi 2p_y^2 = \pi 2p_z^2 < \pi^* 2p_y^0 = \sigma 2p_x^2$

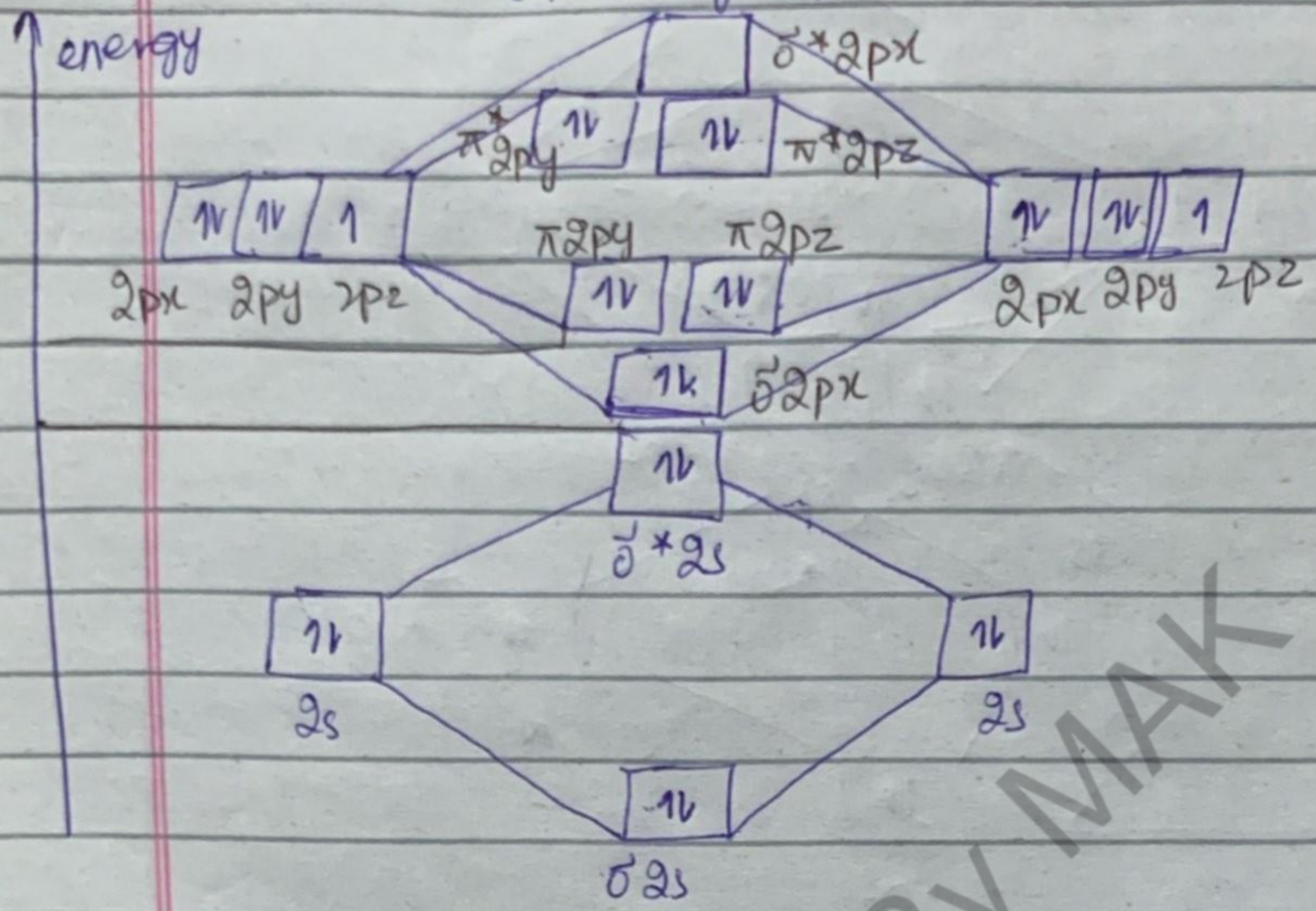
$\pi^* 2p_z^0 < \sigma^* 2p_x^2$

$\Rightarrow \sigma 1s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2 < 2\pi p_y^2 = \pi 2p_z^2 < \sigma 2p_x^2$

$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_x < \pi 2p_y = \pi 2p_z < \pi^* 2p_y = \pi^* 2p_z < \sigma^* 2p_x$

Formation of F_2 :-

F^{9}_{2} $1s^{\uparrow\downarrow}$ $2s^{\uparrow\downarrow}$ $2p_x^{\uparrow\downarrow}$ $2p_y^{\uparrow\downarrow}$ $2p_z^{1}$



Bond energy :- $\frac{8-6}{2} = 2/2 = 1$

F_2 atom have signle bond b/w them.

Magnesium :-

They are diamagnetic.

EC of MOT :-

$\sigma 1s^2 < \sigma^* 1s^2 < \sigma 2s^2 < \sigma^* 2s^2 < \sigma 2p_x^2 < \pi 2p_y^2 = \pi 2p_y^2 < \pi^* 2p_y^2 = \pi^* 2p_y^2$

Application of H-bonding :-

(1) Thermodynamic propties are effect by H-bonding i.e; B.P, M.P, heat of vap, Density.

(2) Solubility of molecules depend on H-bond.
→ All compounds having H-bond dissalve in water.

Q- why alcohol is soluble in H_2O? } bcz of
Q- why carboxylic acid soluble in H_2O? } H_2O

③ cleaning action of soap and detergent is due to the Hydrogen-bonding.

④ Paint and dyes → adhesive property

⑤ clothing → wool, Silk, cotton on basic of H-bonding.

⑥ Food material → carbohydrates dissolve in water.

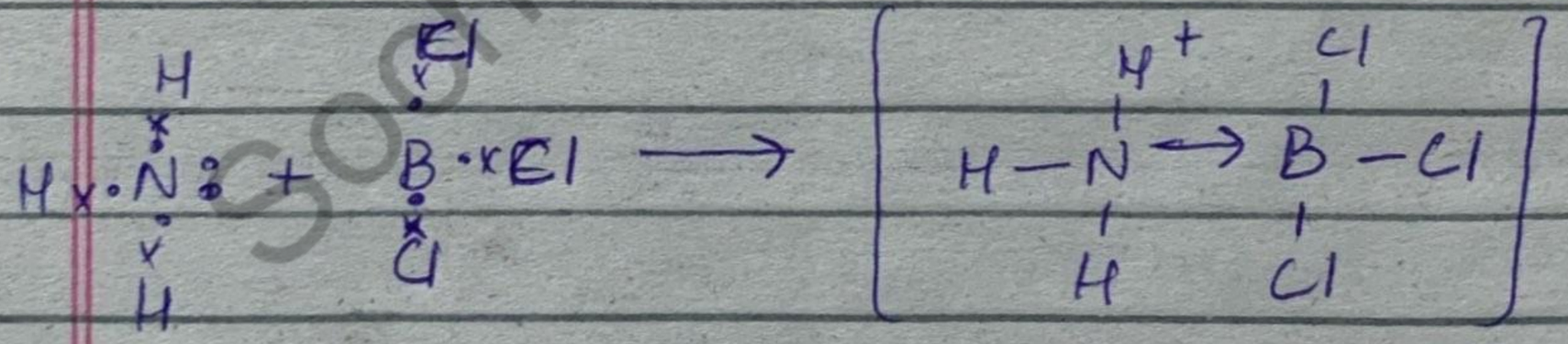
⑦ Biological molecules → DN

Alcohol is soluble in water because it can form hydrogen bondwith water through it's OH group.

Carbonylic acid are souble in water because they have -OH and C=O which makes stronger bond with H_2O molecule.

Assessment 3.3 ⇒

①



②